Appendix 1

I U C L I D

Data Set

Existing Chemical	:	ID: 98-11-3
CAS No.	:	98-11-3
EINECS Name	:	benzenesulphonic acid
EC No.	:	202-638-7
TSCA Name	:	benzenesulfonic acid
Producer related part		
Company	:	Notox
Creation date	:	14.04.2003
Substance related part		
Company	:	Notox
Creation date	:	14.04.2003
Status	:	
Memo	:	
Printing date	:	10.05.2004
Revision date	:	
Date of last update	:	28.04.2004
Number of pages	:	17
Chapter (profile)	:	Chapter: 2, 3, 4, 5, 9
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value : = 43 - 44 °C
Sublimation :
Method :
Year : 1996
GLP :
Test substance :

Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
04.06.2003 (1)

Value : = 50 - 51 °C
Sublimation :
Method :
Year : 2000
GLP :
Test substance :

Remark : Also reported: 65-66 °C for anhydrous and 43-44 °C for sesquihydrate.
Test substance : CAS 98-11-3 (benzenesulphonic acid), anhydrous.
Reliability : (2) valid with restrictions
04.06.2003 (2)

Value : = 89 °C
Sublimation :
Method : other: calculated
Year :
GLP :
Test substance :

Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
07.07.2003 (3)

2.2 BOILING POINT

Value : 171 - 172 °C at .13 hPa

Remark : Using NOMO5 (Mitre Corporation, Version 2.0, 12/4/87), this measured boiling point is estimated to amount to 403 deg C at atmospheric pressure.
Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
19.04.2004 (4)

Value : = 319 °C at 1013 hPa
Decomposition :
Method : other: calculated
Year :
GLP :
Test substance :

Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
28.04.2003 (3)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .0000000022 - .0000047 hPa at 20 °C
Decomposition	:	
Method	:	OECD Guide-line 104 "Vapour Pressure Curve"
Year	:	2004
GLP	:	yes
Test substance	:	
Remark	:	The lower value was calculated from the boiling temperature resulting from the NOMO5 estimation on the measured boiling temperature. The higher value was calculated from the boiling temperature from EPISuite.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(1) valid without restriction

28.04.2004 (5)

Value	:	= .0000228 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

28.04.2003 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	= -1.17 at °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

24.04.2003 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	.7 at 25 °C

Description	:	
Stable	:	
Deg. product	:	
Method	:	
Year	:	2000
GLP	:	
Test substance	:	

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

04.06.2003 (2)

Solubility in	:	Water
Value	:	= 689.5 g/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

Memo	:	Calculated pKa
Remark	:	The pKa was calculated to be -2.80.

Reliability : (2) valid with restrictions
24.04.2003 (6)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000005569 cm³/(molecule*sec)
Degradation	:	= 50 % after 19.2 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	

Remark :

```
AOP Program (v1.90) Results:
==========================
SMILES : O=S(=O)(O)c(cccc1)c1
CHEM   : Benzenesulfonic acid
MOL FOR: C6 H6 O3 S1
MOL WT : 158.17
------------------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
-------
Hydrogen Abstraction       =  0.0000 E-12 cm3/molecule-sec
Reaction with N, S and -OH =  0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds   =  0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =  0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings =  0.4169 E-12 cm3/molecule-sec
Addition to Fused Rings    =  0.0000 E-12 cm3/molecule-sec

  OVERALL OH Rate Constant =  0.5569 E-12 cm3/molecule-sec
  HALF-LIFE =    19.207 Days (12-hr day; 1.5E6 OH/cm3)
..........................  ** Designates Estimation(s) Using ASSUMED Value(s)
------------------- SUMMARY (AOP v1.90): OZONE REACTION ----------------
----

            ******  NO OZONE REACTION ESTIMATION ******
            (ONLY Olefins and Acetylenes are Estimated)
```

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C

Remark	:	Benzene sulphonic acid does not contain any hydrolysable groups. It only ionizes in water. (Basic chemical knowledge)
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

19.04.2004

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

Type of measurement	:	other: concentration at possibly contaminated sites
Media	:	surface water
Concentration	:	
Method	:	sequential solid-phase extraction followed by ion-pair liquid chromatography coupled to electrospray ionisation-mass spectrometry
Method	:	Aliquots of coastal water from two submarine outfalls located at the river mouths of the Besos and the Llobregat near Barcelona were analysed by means of sequential solid-phase extraction followed by ion-pair liquid chromatography coupled to electrospray ionisation-mass spectrometry. Samples were taken bimonthly from March 1999 - July 2000. Nine samples were taken in each specific point.
Result	:	Only in May 1999 a concentration of 1.81-5.35 ng/ml of benzenesulphonic acid was detected in Barcelona coastal waters; the other months amounts were below the limit of detection.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(2) valid with restrictions

24.04.2003 (7)

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: calculated
Year	:	
Remark	:	

Level III Fugacity Model (Full-Output):

==========

Chem Name : Benzenesulfonic acid
Molecular Wt: 158.17
Henry's LC : 2.52e-009 atm-m3/mole (Henrywin program)
Vapor Press : 0.000312 mm Hg (Mpbpwin program)
Liquid VP : 0.00133 mm Hg (super-cooled)
Melting Pt : 88.8 deg C (Mpbpwin program)
Log Kow : -1.17 (Kowwin program)
Soil Koc : 0.0277 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	2.62e-006	461	0
Water	99.8	360	1000
Soil	0.00083	360	0
Sediment	0.166	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.38e-017	1.35e-005	8.97e-005	1.35e-006	8.97e-006
Water	2.72e-014	658	342	65.8	34.2
Soil	8.37e-018	0.00547	0	0.000547	0
Sediment	2.27e-014	0.274	0.0114	0.0274	0.00114

Persistence Time: 342 hr
Reaction Time: 520 hr
Advection Time: 1e+003 hr
Percent Reacted: 65.8
Percent Advected: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 461
Water: 360
Soil: 360
Sediment: 1440
Biowin estimate: 3.014 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : CAS 98-11-3 (benzenesulphonic acid).
Reliability : (2) valid with restrictions
11.07.2003 (3)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 200 mg/l related to COD (Chemical Oxygen Demand)
related to
Deg. product :
Method : other: not indicated
Year : 1976
GLP : no
Test substance :

Method : INOCULUM
- Inoculum: 100 mg/L adapted activated sludge
- Source: sewage plant
- Preparation of inoculum: daily 200 ml is separated from the 1L solution and after sedimentation the residue (200 ml) is diluted with tap water, 600 mg/L starch or glucose, 600 mg/L peptone and 25 ml phosphate buffer pH 7.2 and the tested compound; the concentration of test substance is gradually increased to 200 mg/L COD after 20 days

TEST SYSTEM
- Preparation of test solution: test substance is dissolved in medium
- Initial test substance concentration: 200 mg/L COD
- Culturing apparatus: beakers

- Number of culture flasks per concentration: 1 for test substance + inoculum + medium, 1 blank with inoculum and medium only
- Aeration: no
- Test duration: at least 120 h
- Sampling: once or twice daily
- Analytical parameter: COD

TEST CONDITIONS
- Composition of mineral solution: 27.5 mg CaCl2, 22.5 mg MgSO4.7H2O, 0.25 mg ferric chloride.6H2O, 50 mg ammonium sulphate, 20 ml of phosphate buffer (pH 7.2) and 100 ml tap water in distilled water
- Test temperature: 20 ± 3 °C

REFERENCE SUBSTANCE: 200 mg/L aniline based on COD

Result : Percentage biodegradation corrected for blank: 98.5 based on COD.
Rate of biodegradation: 10.6 mg COD/g/h.

REFERENCE SUBSTANCE
Percentage biodegradation corrected for blank: 94.5 based on COD.
Rate of biodegradation: 19.0 mg COD/g/h.

Test substance : CAS 98-11-3 (benzenesulphonic acid), purity not indicated.

Reliability : (4) not assignable
1. The information is limited to the above mentioned.
2. The study is performed with adapted sludge, which is not allowed according to OECD guidelines.

08.07.2003 (8)

Type : aerobic
Inoculum : other: soil microorganisms
Concentration : 100 mg/l related to Test substance
related to
Deg. product :
Method : other: not indicated
Year : 1966
GLP : no
Test substance :

Method : INOCULUM/TEST ORGANISM
- Inoculum: 1.0 ml of 1% suspension of Niagara silt loam

TEST SYSTEM
- Initial test substance concentration: 45.5 mg C/L
- Culturing apparatus: 45 mm diameter X 80 mm high screw-cap bottles containing 40 ml of medium
- Number of culture flasks per concentration: 2 for test substance + inoculum; 2 for test substance + inoculum + HgCl2; 2 for 1% glucose controls
- Measuring equipment: Beckman spectrophotometer
- Test duration: 64 days
- Sampling: samples were taken after mixing, at intervals of 3 to 6 hours and at 1, 2, 4, 8, 16, 32 and 64 days after inoculation
- Analytical parameter: absorbance at 264 nm relative to soil-medium mixture without chemical

TEST CONDITIONS
- Composition of mineral solution: 1.6 g K2HPO4, 0.40 g KH2PO4, 0.50 g NH4NO3, 0.20 g MgSO4.7H2O, 25 mg CaCl2.2H2O, 2.3 mg FeCl3.6H2O in 1 L of distilled water
- Test temperature: 25 °C

Result : The time necessary for complete degradation was established to be 16 days. The degradation was due to biological activity, because no

decreased absorbance was seen in vessels with HgCl2.

Test substance : CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Reliability : (4) not assignable
The information was limited to the above mentioned.

22.04.2003 (9)

Type : aerobic
Inoculum :
Deg. product :
Method :
Year : 1980
GLP :
Test substance :

Remark : Two hundred sixty of the existing chemicals listed by MITI have been tested for biodegradability; a structure-activity relationship could be deduced for some groups.
Benzenesulphonic acid is reported to be degradable, although the presence of the sulfonic acid-group was indicated to decrease the degradability of aromatic substances.
Test substance : CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Reliability : (4) not assignable
03.06.2003 (10)

Type : anaerobic
Inoculum : other: aquifer microorganisms
Concentration : .2 mmol/l related to Test substance
related to
Contact time : 13 month
Degradation : (±) % after
Result :
Deg. product :
Method : other: not indicated
Year : 1989
GLP : no data
Test substance :

Remark : The test substance was inoculated with aquifer slurry from two sites near a municipal landfill: a methanogenic site (TOC 288 mg/L and sulfate concentration < 0.1 mM) and a sulfate reducing site (TOC 14.4 mg/L and sulfate concentration 2.1 mM). Experiments were performed in the dark at room temperature in duplicate with sterilised aquifer slurries as control. Disappearance of the test substance was analysed by reversed-phase HPLC with UV detection at 264 nm.

Results:
Sulphate-reducing slurry (0, 13 months): 205, 198 µM
Methanogenic slurry (0, 13 months): 204, 196 µM
Test substance : CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Conclusion : No biodegradation was observed for p-hydroxybenzenesulphonic acid.
Reliability : (4) not assignable
22.04.2003 (11)

Type : anaerobic
Inoculum : other: laboratory-made sludge
Concentration : 100 mg/l related to DOC (Dissolved Organic Carbon)
related to
Deg. product :
Method : other: not indicated
Year : 1999
GLP : no data

Test substance	:	
Remark	:	Benzenesulphonic acid was anaerobically incubated with 10 ml of laboratory-made sludge suspension (TOC 158.6 mg/L) at 37 °C for 8 weeks. The gas volume produced was very similar to that of the blank and the test substance was classified as persistent. Benzenesulphonic acid at the concentration used (100 mgC/L) was slightly inhibitory (<=25%) to the microorganisms used. Benzene sulphonic acid is a persistent chemical under the anaerobic degradation conditions as employed in this test.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid), purity analytical grade.
Reliability	:	(4) not assignable

03.06.2003 (12)

Type	:	
Inoculum	:	other: OS-1 bacteria
Deg. product	:	
Method	:	other: not indicated
Year	:	1986
GLP	:	no data
Test substance	:	
Remark	:	A pure culture of OS-1 bacteria isolated to utilise 2-aminobenzenesulphonate as sole carbon source also degraded benzenesulphonate and 4-methylbenzenesulphonate. The respective specific growth rates are 0.11, 0.19 and 0.07 h-1.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Reliability	:	(4) not assignable Only a summary of study is reported.

03.06.2003 (13)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	other
Species	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 1120000
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	other
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 963000
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: green algae
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	g/l
EC50	:	= 502
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Test substance	:	CAS 98-11-3 (benzenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1100 mg/kg bw
Species	:	rat
Strain	:	other: Carworth-Wistar
Sex	:	male
Number of animals	:	5
Vehicle	:	
Doses	:	
Method	:	other: not indicated
Year	:	1962
GLP	:	no
Test substance	:	
Method	:	TEST ANIMALS - Source: in-house colony - Age: 4-5 weeks - Number: 5/dose - Weight at study initiation: 90-120 g ADMINISTRATION - Doses: a logarithmic series of single doses was used differing by a factor of two - Concentration administered: undiluted EXAMINATIONS: mortality during an observation period of 14 days STATISTICAL METHOD: method of Thompson using the Tables of Weil
Result	:	MORTALITY - Number of deaths at each dose: not indicated (only LD50 is reported)
Test substance	:	CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Conclusion	:	The LD50 is 0.89 (0.36-3.21 ml/kg bw), which is equivalent to 1104 mg/kg bw (d = 1.24 g/cm3).
Reliability	:	(2) valid with restrictions Doses used and mortality data are not reported.

07.07.2003 (14)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	other
Value	:	
Species	:	rat
Strain	:	
Sex	:	
Number of animals	:	6
Vehicle	:	
Doses	:	concentrated vapour
Exposure time	:	
Method	:	other: not indicated
Year	:	1962
GLP	:	no
Test substance	:	

Method	:	TEST ANIMALS - Number of animals: 6 males or females ADMINISTRATION Exposure to concentrated vapour is continued for time periods in a logarithmic series with a ratio of two extending from 1/4 to 8 hours, until the inhalation period killing about half the number of rats within 14 days of observation period is defined. - Type or preparation of test condition: For exposures of 10, 5 or 2 minutes a static technique was used by saturating the air with 50-100 g of test substance for 24 hours in a closed chamber. For longer periods a flowstream of saturated vapour was used. EXAMINATIONS: mortality
Result	:	Rats exposed for 8 hours: half the number of rats were killed within 14 days.
Test substance	:	CAS 98-11-3 (benzenesulphonic acid), purity not indicated.
Reliability	:	(3) invalid No guideline study. Amount of test substance that the animals were exposed to is not known.

04.06.2003 (14)

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	TA97, TA98, TA100 and TA1535
Test concentration	:	0, 100, 333, 1000, 3333, 6667 (without activation) and 10000 (with activation) µg/plate
Cytotoxic concentr.	:	> 10000 µg/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	other: not indicated
Year	:	1988
GLP	:	no data
Test substance	:	
Method	:	TEST SYSTEM - Species/cell type: TA97, TA98, TA100 and TA1535

- Deficiency: histidine
- Metabolic activation system: liver S9 fraction (Aroclor 1254-induced) from rats (10 and 30%) and hamsters (10 and 30%)

ADMINISTRATION
- Dosing: 0, 100, 333, 1000, 3333, 6667 (without activation) and 10000 (with activation) µg/plate
- Number of replicates: 3
- Application: preincubation assay
- Positive controls: 2-aminoanthracene (all strains with S9); 4-nitro-o-phenylenediamine (TA98 without S9); sodium azide (TA100 and TA1535 without S9); 9-aminoacridine (TA97 without S9)
- Negative control: DMSO
- Pre-incubation time: 20 min

CRITERIA FOR EVALUATING RESULTS
- Statistical method: Margolin (1981) if result is positive

Result : GENOTOXIC EFFECTS
- With metabolic activation (rat): negative
- With metabolic activation (hamster): negative
- Without metabolic activation: negative

PRECIPITATION CONCENTRATION: 10000 µg/L

CYTOTOXIC CONCENTRATION
- With metabolic activation: >10000 µg/L
- Without metabolic activation: >10000 µg/L

Test substance : CAS 98-11-3 (benzenesulphonic acid), purity >=97%.

Reliability : (2) valid with restrictions
Peer-reviewed, standard article.

09.05.2003 (15)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

9. References

(1) SAX's Dangerous Properties of Industrial Materials, (Ed. R.J. Lewis Sr., 9th Ed., Van Nostrand Reinhold, NY, 1996, p. 340.

(2) Merck Index, CD-rom 2000.

(3) EPISuite v.3.10, April 2001.

(4) Lindner, O., Ullmann's Encyclopedia of Industrial Chemistry, Ed. W. Gerhartz, 5th Ed., VCH Verlag, A3, 1985, p.515, 517-518.

(5) NOTOX BV, Calculation of the vapour pressure of benzenesulphonic acid, Project 408847, 2004

(6) Pallas 2.1, 1994/95.

(7) Alonso MC; Pocurull E; Marce RM; Borrull F; Barcelo D; Monitoring of aromatic monosulfonic acids in coastal waters by ion-pair liquid chromatography followed by electrospray-mass spectrometric detection; Environmental Toxicology and Chemistry 21(10): 2059-2066, 2002.

(8) Pitter, P., Determination of biological degradability of organic substances, Water Res. 10: 231-235, 1976.

(9) Alexander, M; Lustigman, BK; Effect of chemical structure on microbial degradation of substituted benzenes; J. Agric. J. Food Chem. 14: 410-3, 1966.

(10) Kawasaki, M.; Experiences with the test scheme under the chemical control law of Japan: an approach to structure-activity correlations; Ecotoxic. Environ. Safety 4: 444-54, 1980.

(11) Kuhn, EP; Suflita, JM; Anaerobic biodegradation of nitrogen-substituted and sulfonated benzene aquifer contaminants; Waste Hazard. Mater. 6 (2): 121-33, 1989.

(12) Kawahara K(a); Yakabe Y; Ohide T; Kida K; Evaluation of laboratory-made sludge for an anaerobic biodegradability test and its use for assessment of 13 chemicals; Chemosphere 39(12): 2007-2018, 1999.

(13) Thurnherr, T; Köhler, T; Cook, AM; Leisinger, T; Microbial degradation of benzenesulfonic acid and its derivatives; 44th Annual meeting of the Schweizerische Gesellschaft fuer Mikrobiologie (Swiss Soc. of Microbiology), Geneva, Switzerland, Apr. 11-13, 1985. Experientia (Basel): 42(1) 1986. 96.

(14) Smythe, HF; Carpenter, CP; Weil, CS; Pozzani, UC; Striegel, JA; American Ind. Hygiene Association Journal 23: 95-107, 1962.

(15) Zeiger, E; Anderson, B; Haworth, S; Lawlor, T; Mortelmans, K; Speck, W; Salmonella mutagenicity tests: III. Results from the testing of 255 chemicals, Environmental Mutagenesis 9 (Suppl.9): 1-110, 1988.

Appendix 2

I U C L I D

Data Set

Existing Chemical	:	ID: 104-15-4
CAS No.	:	104-15-4
EINECS Name	:	toluene-4-sulphonic acid
EC No.	:	203-180-0
TSCA Name	:	Benzenesulfonic acid, 4-methyl-
Molecular Formula	:	C7H8O3S

Producer related part

Company	:	Notox
Creation date	:	25.06.2003

Substance related part

Company	:	Notox
Creation date	:	25.06.2003
Status	:	
Memo	:	
Printing date	:	22.04.2004
Revision date	:	
Date of last update	:	22.04.2004
Number of pages	:	20
Chapter (profile)	:	Chapter: 2, 3, 4, 5, 9
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

2.1 MELTING POINT

Value	:	106 - 107 °C
Sublimation	:	
Method	:	
Year	:	2000
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), anhydrous.
Reliability	:	(2) valid with restrictions
07.07.2003		(1)

Value	:	107 °C
Sublimation	:	
Method	:	
Year	:	1996
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions
07.07.2003		(2)

Value	:	102 °C
Sublimation	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions
07.07.2003		(3)

2.2 BOILING POINT

Value	:	140 °C at 26.7 hPa
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions
07.07.2003		(1) (2)

Value	:	332 °C at 1013 hPa
Decomposition	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions
07.07.2003		(3)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	.0000039 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	-.62 at °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	ca. 670 g/l at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	
Year	:	2000
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (1)

Solubility in	:	Water
Value	:	202.3 g/l at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	

pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Remark	:	An experimental value of 620 g/L is reported. (original source: Budavari, S. (1989))
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

Memo	:	Calculated pKa
Remark	:	The pKa was calculated to be -2.58.
Reliability	:	(2) valid with restrictions

07.07.2003 (4)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	= .0000000000013643 cm³/(molecule*sec)
Degradation	:	= 50 % after 7.8 day(s)
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	

Remark :

AOP Program (v1.90) Results:
==========
SMILES : O=S(=O)(O)c(ccc(c1)C)c1
CHEM : Benzenesulfonic acid, 4-methyl-
MOL FOR: C7 H8 O3 S1
MOL WT : 172.20
---------- SUMMARY (AOP v1.90): HYDROXYL RADICALS ----------
Hydrogen Abstraction = 0.1360 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.1400 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 1.0883 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 1.3643 E-12 cm3/molecule-sec
HALF-LIFE = 7.840 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 94.080 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.90): OZONE REACTION ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions

07.07.2003 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C

Remark	:	p-Toluenesulphonic acid does not contain any hydrolysable groups. It only ionizes in water. (Basic chemical knowledge)
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(2) valid with restrictions

19.04.2004

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: calculated
Year :

Remark :

Level III Fugacity Model (Full-Output):
==========
Chem Name : Benzenesulfonic acid, 4-methyl-
Molecular Wt: 172.2
Henry's LC : 2.78e-009 atm-m3/mole (Henrywin program)
Vapor Press : 9.57e-005 mm Hg (Mpbpwin program)
Liquid VP : 0.000549 mm Hg (super-cooled)
Melting Pt : 102 deg C (Mpbpwin program)
Log Kow : -0.62 (Kowwin program)
Soil Koc : 0.0984 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	3.18e-006	188	0
Water	99.8	360	1000
Soil	0.000914	360	0
Sediment	0.167	1.44e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	1.54e-017	4.01e-005	0.000109	4.01e-006	1.09e-005
Water	2.76e-014	658	342	65.8	34.2
Soil	9.28e-018	0.00603	0	0.000603	0
Sediment	2.3e-014	0.275	0.0114	0.0275	0.00114

Persistence Time: 342 hr
Reaction Time: 520 hr
Advection Time: 1e+003 hr
Percent Reacted: 65.8
Percent Advected: 34.2

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 188.2
Water: 360
Soil: 360

Sediment: 1440
Biowin estimate: 2.886 (weeks)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Test substance : CAS 104-15-4 (p-toluenesulphonic acid).
Reliability : (2) valid with restrictions
11.07.2003 (3)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : activated sludge, industrial, adapted
Concentration : 100 mg/l related to Test substance
related to
Contact time :
Degradation : 90 (±) % after 24 hour(s)
Result :
Deg. product :
Method : other: activated sludge degradability test
Year : 1988
GLP : no data
Test substance :

Method : Aeration, neutral pH, 10 day adaptation, parameter: TOC
Result : 90% TOC removal
Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.
Reliability : (4) not assignable
The information was limited to the above mentioned.
26.06.2003 (5)

Type : aerobic
Inoculum : activated sludge, adapted
Concentration : 200 mg/l related to COD (Chemical Oxygen Demand)
related to
Deg. product :
Method : other: not indicated
Year : 1976
GLP : no
Test substance :

Method : INOCULUM
- Inoculum: 100 mg/L adapted activated sludge
- Source: sewage plant
- Preparation of inoculum: daily 200 ml is separated from the 1L solution and after sedimentation the residue (200 ml) is diluted with tap water, 600 mg/L starch or glucose, 600 mg/L peptone and 25 ml phosphate buffer pH 7.2 and the tested compound; the concentration of test substance is gradually increased to 200 mg/L COD after 20 days

TEST SYSTEM

- Preparation of test solution: test substance is dissolved in medium
- Initial test substance concentration: 200 mg/L COD
- Culturing apparatus: beakers
- Number of culture flasks per concentration: 1 for test substance + inoculum + medium, 1 blank with inoculum and medium only
- Aeration: no
- Test duration: at least 120 h
- Sampling: once or twice daily
- Analytical parameter: COD

TEST CONDITIONS
- Composition of mineral solution: 27.5 mg CaCl2, 22.5 mg MgSO4.7H2O, 0.25 mg ferric chloride.6H2O, 50 mg ammonium sulphate, 20 ml of phosphate buffer (pH 7.2) and 100 ml tap water in distilled water
- Test temperature: 20 ± 3 °C

REFERENCE SUBSTANCE: 200 mg/L aniline based on COD

Result : Percentage biodegradation corrected for blank: 98.7 based on COD.
Rate of biodegradation: 8.4 mg COD/g/h.

REFERENCE SUBSTANCE
Percentage biodegradation corrected for blank: 94.5 based on COD.
Rate of biodegradation: 19.0 mg COD/g/h.

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.

Reliability : (4) not assignable
1. The information is limited to the above mentioned.
2. The study is performed with adapted sludge, which is not allowed according to OECD guidelines.

08.07.2003 (6)

Type : aerobic
Inoculum :
Concentration : .6 g/l related to COD (Chemical Oxygen Demand)
related to
Contact time :
Degradation : 44 (±) % after
Result :
Deg. product :
Method : other: not indicated
Year : 1972
GLP : no
Test substance :

Remark : COD 1560 mg O2/g
BOD 1030 mg O2/g

Degradation (= reduction of COD): 44%

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity pro analyse.

Reliability : (4) not assignable
The information is limited to the above mentioned.

07.07.2003 (7)

Type : aerobic
Inoculum :
Contact time :
Degradation : > 90 (±) % after 5 day(s)
Result :
Deg. product :
Method : other: not indicated
Year : 1978
GLP : no

Test substance	:	
Remark	:	Organic carbon 450 mg/g ThOD 1672 mg O2/g COD 1480 mg O2/g BOD 380 mg O2/g COD-elimination: >90% after 5 days
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.
Reliability	:	(4) not assignable The information is limited to the above mentioned.
07.07.2003		(8)
Type	:	aerobic
Inoculum	:	
Contact time	:	
Degradation	:	100 (±) % after 5 day(s)
Result	:	
Deg. product	:	
Method	:	other: not indicated
Year	:	1983
GLP	:	no data
Test substance	:	
Remark	:	DOC 360 mg C/g COD 1040 mg O2/g BOD 300 mg O2/g Degradation was 10% after 3 hours and 100% after 5 days.
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity 65%.
Reliability	:	(4) not assignable The information is limited to the above mentioned.
07.07.2003		(9)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Leuciscus idus melanotus (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	> 325
Limit test	:	no
Analytical monitoring	:	no
Method	:	other: not indicated
Year	:	1981
GLP	:	no
Test substance	:	

Method :

TEST ORGANISMS
- Species: Leuciscus idus f. melanotus
- Supplier: Paul Eggers, 2345 Hohenwestedt
- Size/weight/loading: 5.5-6.6 cm/1.5-2.7 g/0.75-1.35 g/L
- Feeding (pretreatment): Tetra Min

STOCK AND TEST SOLUTION AND THEIR PREPARATION
Test substance was dissolved in medium and added to the solution in the aquarium.

DILUTION WATER
- Source: deionised tapwater
- Hardness: 114 mg CaCO3/l
- Ca/Mg ratio: 0.7
- Na/K ratio: 21
- pH (after aeration with fish): 8.0-8.2
- O2: >7 mg/L
- Conductance: <5 µS/cm

TEST SYSTEM
- Test type: static
- Concentrations: 0, 10, 100 and 500 mg/L
- Exposure vessel type: glass aquarium (40x25x30 cm) containing 20 liter of solution
- Number of fish: 10 per replicate, 1 replicate/treatment
- Photoperiod: 12 hours (700 lux)
- Test duration: 96 hours
- Test parameter: mortality
- Observation times: regularly
- Aeration: yes

PHYSICAL MEASUREMENTS
- Measuring times: 0, 2, 24, 48, 72 and 96 hours for pH, dissolved oxygen and temperature
- Test temperature: 20 ± 1 °C
- Dissolved oxygen: 8.5-9.2 mg/L
- pH: 7.5-8.2 (at 500 mg/L 5.7 after 2 hours and still slightly decreased after 24, 48 and 96 hours)

Result :

RESULTS
- Mortality: none
- Other effects: no difference in behaviour compared to control group; macroscopic examination showed no changes

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity 65% in water.
Conclusion	:	The LC50 >500 mg/L, which is equivalent to >325 mg/L (p-toluenesulphonic acid is a 65% solution in water).

Reliability	:	(2) valid with restrictions The method used is predominantly according to OECD203, except that Leuciscus idus melanotus is not a recommended species, only 4 concentrations were tested and no analyses were performed.
Flag	:	Critical study for SIDS endpoint

07.07.2003 (10)

Type	:	other: not indicated
Species	:	Lebistes reticulatus (Fish, fresh water)
Exposure period	:	48 hour(s)
Unit	:	mg/l
LC0	:	> 500
Limit test	:	
Analytical monitoring	:	no data
Method	:	other: not indicated
Year	:	1972
GLP	:	no
Test substance	:	

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity pro analyse.
Reliability	:	(4) not assignable The information is limited to the above mentioned.

07.07.2003 (7)

Type	:	other: not indicated
Species	:	Leuciscus idus (Fish, fresh water)
Exposure period	:	
Unit	:	mg/l
LC0	:	= 200
Limit test	:	
Analytical monitoring	:	no data
Method	:	other: not indicated
Year	:	1978
GLP	:	no
Test substance	:	

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.
Reliability	:	(4) not assignable The information is limited to the above mentioned.

07.07.2003 (8)

Type	:	other
Species	:	
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	= 371000
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	
Species	:	Daphnia magna (Crustacea)
Exposure period	:	

Unit	:	mg/l
EC0	:	> 1625
Analytical monitoring	:	no data
Method	:	other: not indicated
Year	:	1983
GLP	:	no data
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity 65%.
Conclusion	:	EC0 >2500 mg/L, which is equivalent to 1625 mg/L for the substance tested (65%).
Reliability	:	(4) not assignable The information is limited to the above mentioned.

07.07.2003 (9)

Type	:	other
Species	:	Daphnia sp. (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
EC50	:	= 331000
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species	:	other algae: green algae
Endpoint	:	
Exposure period	:	96 hour(s)
Unit	:	g/l
EC50	:	= 178
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid).
Reliability	:	(4) not assignable

07.07.2003 (3)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 1410 mg/kg bw
Species	:	rat
Strain	:	Wistar
Sex	:	male/female
Number of animals	:	5
Vehicle	:	
Doses	:	1250, 1600 and 2000 mg/kg for females and 2000 mg/kg for males
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	1988
GLP	:	yes
Test substance	:	

Method :

TEST ANIMALS:
- Source: Hoechst AG
- Age: male ca. 7 weeks, female ca. 8 weeks
- Number: 5/sex/dose
- Weight at study initiation: male 194-202 g; female 181-196 g

ADMINISTRATION
- Route: oral (gavage)
- Doses: 1250, 1600 and 2000 mg/kg for females and 2000 mg/kg for males
- Volume administered or concentration: 10 ml/kg

EXAMINATIONS: mortality and clinical symptoms several times on day 1 and daily thereafter; body weight weekly; macroscopic examination of animals found dead and sacrificed; post-exposure period was 28 days.

STATISTICAL METHOD: Probit-analysis

Result :

MORTALITY
- Number of deaths at each dose: 2/5, 3/5 and 4/5 at 1250, 1600 and 2000 mg/kg for females and 2/5 at 2000 mg/kg for males
- Time of death: on day 1, except for 1 animal at 1600 mg/kg died on day 13

BODY WEIGHT: decreased body weight during post-exposure period.

MAIN CLINICAL SIGNS:
Hypoactivity, hunched posture, emaciation, irregular breathing were observed in all animals from all dose groups on day 1 and reversible within 3 days for males at 2000 mg/kg. In males at 2000 mg/kg some of the symptoms re-occurred in 1 or 2 animals after 14 days. For females at 1250 mg/kg the above symptoms were reversible within 2 days. For females at 1600 and 2000 mg/kg some of the symptoms were irreversible in 1-2 animals.
Abnormal gait, ptosis and piloerection were seen in several animals from all dose groups on day 1. Symptoms were reversible within 2 days for males at 2000 mg/kg and for females at 1250 mg/kg; some symptoms re-occurred within the 28-day observation period. For females at 1600 and 2000 mg/kg ptosis, piloerection and abnormal gait were observed during the 28 days observation period.

NECROPSY FINDINGS:
Red discolouration of the GI tract filled with blood, white discolouration of the mucosa of the stomach and intestine, pale adrenals, growing together of stomach and nearby organs, stomach haemorrhages and abdomen filled with fluid (in animals that died spontaneously).

SEX-SPECIFIC DIFFERENCES: none

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity >98%.
Reliability : (1) valid without restriction
02.04.2004 (11)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : 500 mg
Exposure : Semiocclusive
Exposure time : 4 hour(s)
Number of animals : 1
Vehicle : physiol. saline
PDII :
Result : corrosive
Classification : corrosive (causes burns)
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year : 1988
GLP : yes
Test substance :

Method : TEST ANIMALS
- Strain: New Zealand white rabbit
- Sex: not indicated
- Age: ca. 3-5 months
- Weight at study initiation: 2.0-2.6 kg
- Number of animals: 1 (3 animals were exposed for 3 minutes)

ADMINISTRATION/EXPOSURE
- Preparation of test substance: 500 mg wetted with 0.1 ml 0.9% saline
- Area of exposure: 6.25 cm2
- Occlusion: semiocclusion
- Removal of test substance: with water after exposure

EXAMINATIONS
- Scoring system: Draize
- Observation times: 30-60 minutes, 24, 48 and 72 hours, and 7 days after exposure for 4 hours exposure only

Result : 4-hour exposure:
AVERAGE SCORE (24-72 h)
- Erythema: 3.7
- Edema: 2

REVERSIBILITY: not reversible within 7 days

OTHER EFFECTS: dry, fissured skin, eschar formation, brown discolouration; scar formation and open wound after 7 days

3-minute exposure:
AVERAGE SCORE (24-72 h)
- Erythema: 0.6
- Edema: 0

REVERSIBILITY: within 72 hours

OTHER EFFECTS: brown discolouration

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity >98%.
Reliability : (1) valid without restriction
22.03.2004 (12)

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	Sub-acute
Species	:	rat
Sex	:	male/female
Strain	:	Wistar
Route of admin.	:	oral unspecified
Exposure period	:	28 days
Frequency of treatm.	:	daily; 7 times/week
Post exposure period	:	
Doses	:	0, 4, 20, 100, 500 mg/kg bw/d
Control group	:	yes
NOAEL	:	> 500 mg/kg bw
Method	:	OECD Guide-line 407 "Repeated Dose Oral Toxicity - Rodent: 28-day or 14-d Study"
Year	:	1990
GLP	:	yes
Test substance	:	
Result	:	In the highest dose group urine was acidic in both sexes and in males a higher saliva production at the end of the study was observed.
Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity not indicated.
Conclusion	:	The findings observed at 500 mg/kg are not considered to be toxicologically relevant. NOEL = 100 mg/kg.
Reliability	:	(4) not assignable Secondary literature. The information given was limited to the above mentioned.

22.04.2004 (13)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Ames test
System of testing	:	Salmonella typhimurium TA98, TA100, TA1535, TA1537 and TA1538
Test concentration	:	0, 10, 100, 500, 1000 and 5000 µg/plate

Cytotoxic concentr.	:	>5000 µg/plate
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 471
Year	:	1988
GLP	:	yes
Test substance	:	

Method :

TEST SYSTEM
- Species/cell type: Salmonella typhimurium TA98, TA100, TA1535, TA1537 and TA1538
- Deficiency: histidine
- Metabolic activation system: Aroclor 1254 rat liver S9-mix

ADMINISTRATION
- Dosing: 0, 10, 100, 500, 1000 and 5000 µg/plate
- Number of replicates: 3
- Application: plate incorporation
- Positive control groups: sodium azide (without S9; TA1535 and TA100); 9-aminoacridine (without S9; TA1537); 2-nitrofluorene (without S9; TA1538 and TA98); 2-aminofluorene (with S9; TA1538 and TA98).
- Negative control group: distilled water

DEVIATIONS FROM GUIDELINE: no positive controls were used for TA100, TA1535 and TA1537 with metabolic activation; however, the number of revertants is very low.

Result :

GENOTOXIC EFFECTS
- With metabolic activation: negative
- Without metabolic activation: negative

PRECIPITATION CONCENTRATION: >5000 µg/plate

CYTOTOXIC CONCENTRATION
- With metabolic activation: >5000 µg/plate
- Without metabolic activation: >5000 µg/plate

Test substance	:	CAS 104-15-4 (p-toluenesulphonic acid), purity >98%.
Reliability	:	(1) valid without restriction 1. As no E-coli strain was included in the study design some base-pair substitutions may remain undiscovered. 2. The number of cells/culture were not specified.

07.07.2003 (14)

Type	:	Chromosomal aberration test
System of testing	:	V79 Chinese hamster cells
Test concentration	:	0, 200, 600 and 1902 µg/ml
Cytotoxic concentr.	:	>1902 µg/ml
Metabolic activation	:	with and without
Result	:	negative
Method	:	OECD Guide-line 473
Year	:	1988
GLP	:	yes
Test substance	:	

Method :

TEST SYSTEM
- Species/cell type: V79 Chinese hamster cells
- Metabolic activation system: Aroclor 1254 induced rat liver S9-mix
- No. of metaphases analyzed: 100

ADMINISTRATION
- Dosing: 0, 200, 600 and 1902 µg/ml
- Number of replicates: 2

- Application: in bidest water
- Positive control group: ethylmethanesulfonate (without S9), cyclophosphamide (with S9)
- Negative control groups: bidest water and untreated
- Pre-incubation time: 24 hours
- Incubation time: 2 hours
- Fixation interval: 6, 18 and 28 hours for 1902 µg/ml and 18 hours for 200 and 600 µg/ml (last 2.5 hours Colcemid was added)

CRITERIA FOR EVALUATING RESULTS
classified as mutagenic if the test substance induces a significantly increased aberration rate as compared with the negative controls with one of the concentrations tested and if there is a reproducible concentration related increase in the aberration rate.

Result : GENOTOXIC EFFECTS
- With metabolic activation: negative
- Without metabolic activation: negative

FREQUENCY OF EFFECTS (excluding gaps)
without S9: 2, 0.5 and 0% at 200, 600 and 1902 µg/ml after 18 hours; 2% at 1902 µg/ml after 28 hours
with S9: 2.5, 2 and 0.5% at 200, 600 and 1902 µg/ml after 18 hours; 0.5% at 1902 µg/ml after 28 hours

PRECIPITATION CONCENTRATION: >1902 µg/ml (= 10 mM)

MITOTIC INDEX: Concentration-related plating efficiency was established in 1000 cells from each of two slides per test group. No influence on mitotic index was observed.

CYTOTOXIC CONCENTRATION
- With metabolic activation: >1902 µg/ml
- Without metabolic activation: >1902 µg/ml

Test substance : CAS 104-15-4 (p-toluenesulphonic acid), purity >98%.

Reliability : (1) valid without restriction

07.07.2003 (15)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

9. References

(1) Merck Index, CD-rom 2000.

(2) SAX's Dangerous Properties of Industrial Materials, (Ed. R.J. Lewis Sr., 9th Ed., Van Nostrand Reinhold, NY, 1996, p. 3195.

(3) EPISuite v.3.10, April 2001.

(4) Pallas 2.1, 1994/95.

(5) Matsui, S.; Y. Okawa & R. Ota, Experience of 16 years' operation and maintenance of the Fukashiba industrial wastewater treatment plant of the Kashima petrochemical complex - II. Biodegradability of 37 organic substances and 28 process wastewaters, Water Sci. Technol. 20: 201-210, 1988.

(6) Pitter, P., Determination of biological degradability of organic substances, Water Res. 10: 231-235, 1976.

(7) Hoechst AG, internal report (07.12.1972).

(8) Hoechst AG, internal report (31.08.1978).

(9) Hoechst AG, internal report, Bericht W82-360 (23.3.1983).

(10) Hoechst AG, Akute Toxizitaet von p-Toluolsulfonsaeure Loesung 65%ig an Goldorfen, Bericht 197/81, 1981.

(11) Hoechst AG, p-Toluolsulfonsaeure: Pruefung der akuten oralen Toxizitaet an der Wistar-Ratte, Bericht 88.1563, 1988.

(12) Hoechst AG, p-Toluolsulfonsäure: Prüfung auf Hautreizung am Kaninchen, Bericht 88.1576, 1988.

(13) Hoechst AG (1990): Internal report No. 90.0037 in IUCLID Dataset Toluene-4-sulphonic acid (CAS No. 104-15-4) on IUCLID CD-ROM, 2000.

(14) Hoechst AG, EXT 8804 p-Toluenesulfonic acid: Reverse mutation assay in vitro Ames test, Bericht 88.0892, 1988.

(15) Hoechst AG, p-Toluolsulfonsaeure: Chromosome aberrations in vitro in V79 chinese hamster cells, Report No. 88.1940, 1988.